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Advanced models for the calculation of capillary attraction in axisymmetric configurations

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ABSTRACT

The proper estimate of capillary attraction is of great importance in many situations, for example the reliability assessment of Micro- Electro-Mechanical Systems (MEMS) with respect to spontaneous adhesion. In spite of many theoretical studies, there is a lack of general methods for obtaining the exact shape of the liquid meniscus between the asperities of rough surfaces. In this paper, a new analytical method is developed for the specific case of axysimmetric configurations. The outcomes of such a method are critically compared with the approximate solution which is usually proposed in the literature. Moreover, an improved simplified method is constructed and validated. Finally, a more general procedure (based on the Finite Element Method) is proposed, with possible application to non-symmetric geometries.

1. Introduction

The reliability of Micro-Electro-Mechanical Systems (MEMS) is a topic of paramount importance for technological advances: proper design and fabrication of micro-devices must ensure the perfect functioning both in standard exercise conditions and in extreme situations. Among the various dangerous phenomena, spontaneous adhesion can seriously compromise the MEMS reliability. Due to the high surface-to-volume ratio, the adhesive forces between parts in contact may exceed the elastic restoring force: in this case, the components remain stuck to each other and the microsystem can be completely unusable. This situation is addressed to in the literature as *stiction*, a neologism coined from *static friction* (see e.g. (Mastragelo and Hsu, 1993) and (Tas et al., 2003)).

Various phenomena can contribute to the adhesion at the nano-scale causing attractive forces between components: the most relevant ones are van der Waals (Delrio et al., 2005) and capillarity forces (Hariri et al., 2007). This research mainly focuses on the latter, caused by liquid menisci capillary condensation which entails the formation of liquid menisci around the contact areas of two neighbouring asperities. The computation of the capillarity forces is subordinated to the evaluation of the shape of the meniscus and the solution of such a problem represents an awkward task. One can follow two different approaches (Payam and Fathipour, 2011) depending on whether or not thermodynamic equilibrium is assumed between the liquid and the surrounding gas. If equilibrium is assumed, the meniscus mean curvature is constant and Kelvin equation holds, which is solvable either in analytical (Stifter et al., 2000) or in numerical (Pakarinen et al., 2005, Chau et al., 2007) way; if no equilibrium is assumed, a formulation based on liquid volume conservation must be considered. Many works refer to this situation (Rabinovich et al., 2005, Mu and Su, 2007, Payam and Fathipour, 2011); however it is more realistic to assume thermodynamic equilibrium since, in a typical situation, menisci between MEMS components are caused by capillarity condensation and there is no way to evaluate the volume of the liquid bridges from which the estimate of the force depends (Butt, 2008).

Whatever option will be taken, the proper evaluation of the capillarity force requires the computation of the geometrical shape of the menisci. In spite of many important theoretical studies (see e.g. (Lian et al., 1993; Melrose, 1966)), there is a lack of general methods to be applied for obtaining the exact configuration of the liquid bridge. The problem has been tackled for simple cases, such as a meniscus between two spheres or between a sphere and a flat. As a matter of fact, those cases are consistently far away from the realistic situation of rough surface, endowed with a random distribution of asperities with generic shape. Nonetheless, it is possible to envisage that satisfactory results could be obtained by replacing the actual geometry of the asperities by means of approximate axisymmetric surfaces. In this ambit, many

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approximations have been proposed, both geometric and numeric, as equal contact angle with the two particles between which the meniscus is formed (Israelachvili, 2011, Lambert et al., 2008, Mu and Su, 2007), same radius for the two spheres (Mu and Su, 2007, Rabinovich et al., 2005), circular arc or paraboloid approximation for the vertical profile of the liquid bridge interface (de Lazzer et al., 1999, Pepin et al., 2000, Stifter et al., 2000): it is demonstrated that circular approximation is suitable in many situations (Pakarinen et al., 2005). Another approximation that usually holds is based on the assumption that the liquid menisci extend much further in the direction parallel to the gap than normal to it (de Boer and de Boer, 2007, Butt, 2008), which is reasonable only when the distance between the particles is quite small. Otherwise, it can lead to a discrepancy between the calculated forces and experimental results because menisci can be stretched along their axis and the assumption does not hold anymore.

In this research, a new predictive analytical tool for the attractive force due to a single meniscus in axisymmetric conditions has been developed, with the aim of obtaining the exact solution for the meniscus shape in the hypothesis of thermodynamic equilibrium. The analytical tool has been obtained by applying, in an innovative way, a mathematical procedure originally proposed in (Kenmotsu, 1980). The results obtained by the exact approach have been critically compared to some quick, though approximate, procedures based on reasonable geometric assumptions: a standard approximate procedure has been considered and a new, refined model has been developed in order to obtain better results. In any case, the aforementioned approximation for normal and parallel sizing has been avoided. Finally, the analytical outcomes have been adopted in order to validate a generic simulation tool based on the numerical simulation of the meniscus mechanical behaviour. Such a tool, which represents another innovative aspect of this paper, has the outstanding merit of possible application to non-axisymmetric geometries.

This paper is organized as follows: Section 2 contains some basic information on capillary attraction; the exact solution for the meniscus shape is summarized in Section 3; the approximate procedures are described in Section 4; Section 5 contains the description of the numerical approach; a certain number of results are reported in Section 6, along with critical comparisons; some conclusions and future prospects are drawn in Section 7.

2. Capillarity

When two micro-particles are close to contact, if the surfaces are lyophilic with respect to a surrounding vapour, some vapour will condense and form a meniscus. The meniscus causes a force that attracts the particles for two reasons: the direct action of the surface tension of the liquid around the periphery of the meniscus and the pressure inside the meniscus, that is reduced as compared to the outer pressure by the capillary pressure ΔP, which acts over the cross-sectional area of the meniscus.

The computation of both these contributions is subordinated to the evaluation of the shape of the meniscus. The solution of such a problem represents a non-trivial task, even in the case of regular asperities.

According to the physical properties of the surface, the meniscus will form the given contact angle θ with the solid surface. The two additional equations describing the thermodynamic equilibrium state of a meniscus are the Young–Laplace equation and the Kelvin equation (Adamson and Gast, 1997). The first one relates the curvature of a liquid interface to the pressure difference ΔP between the two fluid phases. In the self-weight of the meniscus is negligible, the enforcement of the mechanical equilibrium of the interface leads to the Young–Laplace equation:

$$\Delta P = P_l - P_g = \gamma_L \left(\frac{1}{r_1} + \frac{1}{r_2} \right) \equiv \frac{\gamma_L}{r_k} \tag{1}$$

Here, γ_L is the surface tension of the liquid, l and g denote the liquid and the gas respectively, r_1 and $\mathcal{P}$ are the principal radii of curvature that describe the interface, r_k is the *Kelvin radius*. Even if the sign of the radius of curvature is usually defined with respect to the choice of a normal to the surface, in capillarity theory it is common to count the radius positive if the interface is curved towards the liquid. As a result, a spherical liquid droplet with radius R in a gas has $\dot{S}[\mathbf{w}]$ whereas a spherical bubble in a liquid has $r_1 = r_2 = -1/R$.

The Kelvin equation, instead, relates the actual vapour pressure P to the curvature of the surface of the condensed liquid:

$$r_k = \left(\frac{1}{r_1} + \frac{1}{r_2} \right)^{-1} = \frac{\gamma_L Vm}{RT \log(P/P_0)} = \frac{\gamma_L Vm}{RT \log(RH)} \tag{2}$$

where R is the molar gas constant, T the absolute temperature, P_0 the saturation vapour pressure over a planar liquid surface and V_m the molar volume of the liquid. For a typical meniscus with hydrophilic contact angle, $r_1 < 0$, $r_2 > 0$, $r_2 \gg r_1$ and so $1/r_1 + 1/r_2$ is negative: coherently $P < P_0$ and $\log(P/P_0)$ is negative.

Once the geometric configuration of the meniscus has been obtained, straigthforward considerations allow one to obtain the area of the horizontal projection of the wetted region ($A = \pi r_m^2$) and the length of the contact circle ($L = 2\pi r_m$). The (vertical) attraction force exerted on the two surfaces is given by the sum of the following actions: 1) surface tension over the contact length, $\gamma_L L |t_z^u|$, where t_z^u is the vertical component of the unit tangent to the meniscus at the contact point with the solid surface; 2) capillary pressure over the wetted area, $|\gamma_L/r_k|A$.

3. Exact solutions for axisymmetric geometries

The problem of describing analytically surfaces with prescribed mean curvature was tackled and solved in (Kenmotsu, 1980). Such a contribution has been largely overlooked in the ambit of capillary condensation, in spite of its perfect suitability to the problem at hand. In this Section, we prove that the procedure proposed in (Kenmotsu, 1980), if properly adapted, can be used in order to find the analytical solution for the meniscus shape. This is of paramount importance, for a twofold reason: first, the difficulties and inaccuracies of the numerical solutions of the governing differential equation are avoided; second, some specific features, specially regarding unstable behaviour, can be pointed out, contrarily to what can be done with a numerical approach.

Let z be the axis of rotation, as depicted in Fig. 1. If the generating curve in the $x = 0$ plane is expressed in parametric form as $y(s)$, $z(s)$, the principal radii of curvature are:

$$\frac{1}{r_2} = -\frac{z'(s)}{y(s)} \qquad \frac{1}{r_1} = -z''(s)y'(s) + z'(s)y''(s) \tag{3}$$

curvatures are positive if oriented as $\mathbf{n}(s)$, where the normal to the curve is such that the vector product $\mathbf{n}(s) \wedge \mathbf{t}(s) = \mathbf{e}_x$, i.e. is oriented as the out-of-plane x axis. We will henceforth impose the condition $z'(s)^2 + y'(s)^2 = 1$, which identifies s as the arc length.

As will be shown later on, the families of surfaces describing physical menisci are associated with generating curves of the type depicted in Fig. 1 on the left, where the portion of interest is any of the "ribbons" described by the curve and characterized by negative $z'(s)$. The signs adopted in Eq. (3) have been selected to comply with the conventions of the previous section (i.e. radius of curvature directed towards the meniscus).